

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so as that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

*SUB D/ Cont* providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

*d* deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component

spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces;

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Cont. assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces,

deriving the reaction characteristic values for all the component spaces of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules, a reaction characteristic of each of the data molecule being known,

Q. deriving the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

14. (Amended) A molecular reaction characteristic predicting method as set forth in claim 1, which further comprises the steps of:

processing the plurality of data vectors for the data molecules in accordance with a technique of a self-organizing neural network to display the processed result on a reaction characteristic predicting map indicative of reaction characteristics of said plurality of molecules, and

predicting the reaction characteristic of the predicting molecule based on the map.

18. (Twice Amended) A molecular reaction characteristic predicting method comprising the steps of:

describing atomic spherical surfaces, each of which surrounds a corresponding one of atoms of a molecule;

C3 assuming that a portion of each of said atomic spherical surfaces intersecting the atomic spherical surfaces of other atoms of said molecule is an interior spherical surface;

assuming that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier spherical surface, the frontier spherical surface being appeared outside;

providing probe points on each of said atomic spherical surfaces at regular intervals;

deriving a rate of occupied space as a space occupied rate of a corresponding one of said atoms, for each of said atoms;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of said atoms of said molecule, for each of said probe points on said frontier spherical surface of each of said atoms;

deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said atoms, as an electrostatic factor of said corresponding one of said atoms;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said atoms;

deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said atoms, as a steric factor of said corresponding one of said atoms;

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said atoms;

deriving the reaction characteristic values for all the atoms of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules, a reaction characteristic of each of the data molecules being known,

c3 deriving the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and

having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and

predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

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20. (Twice Amended) A computer-readable storage medium having stored a program for predicting a reaction characteristic of a molecule, said program carrying out a process comprising the steps of:

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setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so as

that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

cd. deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of

said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces,

deriving the reaction characteristic values for all the component spaces of a predicting molecule of which a reaction characteristic is to be predicted,

forming a predicting vector having a plurality of vector components selected from the reaction characteristic values of the predicting molecule,

selecting a plurality of data molecules, a reaction characteristic of each of the data molecules being known,

deriving the reaction characteristic values for all the component spaces of each of the data molecules,

forming a data vector for each of the data molecules, the data vector being corresponding to the predicting vector and having a plurality of vector components selected from the reaction characteristic values of each of the data molecules,

estimating a Euclid distance between the predicting vector and each data vector and getting a plurality of Euclid distances between the predicting vector and all the data molecules, and



predicting the reaction characteristic of the predicting molecule to be that the reaction characteristic of the predicting molecule is more similar to a reaction characteristic of a data molecule related to a shorter Euclid distance.

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